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Movement of Kepone (Trade Name) (Chlordecone) Across an Undisturbed Sediment-Water Interface in Laboratory Systems

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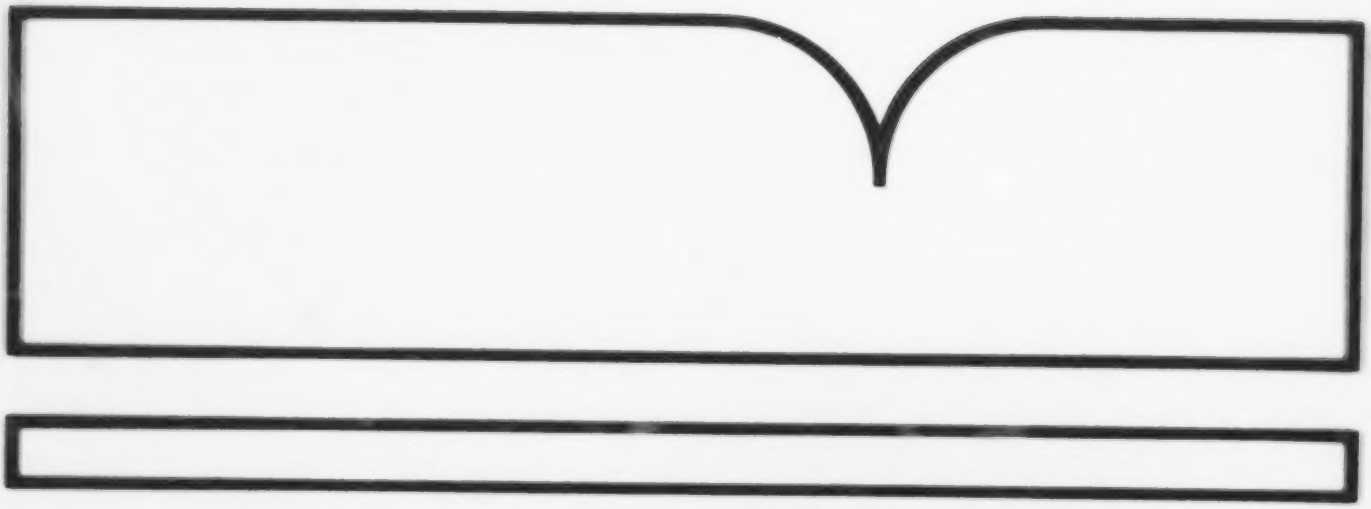

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16. ABSTRACT

The distribution (labeled Kepone was studied in a continuous flow sediment-water microcosm. dict the fate of the compound in an aquatic environment. The sediment fractionated into layers and the sorbed Kepone concentrations were measured to determine toxicant penetration into the sediment. The data were used to test the validity of using a mathematical model based on independent studies of the processes affecting Kepone to predict the distribution of the toxicant in the microcosm sediment and water. The model accurately described the observed Kepone distribution. Microcosms, by simulating the complexity of natural environments, provided a useful tool for evaluating the accuracy of mathematical predictions concerning the distribution of a toxicant in aquatic systems.

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MOVEMENT OF KEPONE® (CHLORDECONE) ACROSS AN UNDISTURBED SEDIMENT-WATER INTERFACE IN LABORATORY SYSTEMS

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Abstract—The distribution of Kepone® (chlordecone) in a sediment bed after various periods of continuous toxicant input to the overlying water column was determined in a laboratory system. Most of the Kepone was found to accumulate in the top 0.6 to 1.5 cm of sediment. A mathematical model was developed to predict Kepone concentrations with depth over time in the sediment. An equilibrium partition coefficient was determined from batch sorption tests and a molecular diffusion coefficient for Kepone was estimated from an empirical relationship between diffusivity and molecular weight. A computed Kepone distribution based on diffusion rates that decreased with depth and with incubation time gave the best fit to the observed data. We attribute the apparently faster rates in the upper sediment to mixing between interstitial and overlying water. Our results illustrate the value of models in conjunction with laboratory studies in defining the interactions of pollutants with sediment beds.

Keywords—Kepone Diffusion Model Sediment

INTRODUCTION

Information on rates of biotic and abiotic degradation, sorption to suspended and bed solids and transport across the sediment-water interface is necessary to predict the fate of xenobiotic chemicals in aquatic environments. Simple laboratory tests, such as studies in shake flasks, enable us to isolate and measure individual fate processes under a variety of experimental conditions. Field studies ultimately test the environmental significance of laboratory results but field validation tests are seldom feasible because of logistical, economic and climatic problems. Microcosms, complex laboratory systems designed to simulate conditions in the field, can be used as surrogates for field studies and to test the environmental significance of laboratory data derived from simpler tests [1-4]. If information from simple laboratory tests can be integrated through the use of a mathematical model to quantitate the fate of a chemical in a complex laboratory system, then that information may be applicable to the environment.

Rodgers et al. [5] studied the fate of naphthalene and lindane in aquatic microcosms, but their data did not support predictions from two different mathematical models. The inadequate predictions were attributed to a lack of information on the movement and degradation of the chemicals in sediments.

Falco et al. [6] used predictive modeling to show that second-order kinetic expressions for biotic and abiotic degradation, coupled with laboratory-derived rate constants, could accurately predict the fate of malathion in a microcosm. Marshall and Roberts [7] found that estimates from simple laboratory tests of adsorption, biodegradation, photolysis and uptake of fenitrothion by fish provided sufficient data for a mathematical model to predict the fate of fenitrothion in a farm pond. Blau and Neeley [8] described similar studies with Dursban®.

These studies emphasized the importance of assessing the fate of xenobiotic chemicals in systems containing sediment beds, whether those sys-

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Mention of trade names does not constitute endorsement by the U.S. Environmental Protection Agency.

tems are microcosms or in the field. In an effort to characterize more completely the transport processes at the sediment-water interface, we measured the distribution of Kepone in a laboratory system containing an undisturbed sediment bed. We also developed a simple mathematical model that describes the diffusion of hydrophobic chemicals into sediment and the partitioning of chemicals to sediment. We selected Kepone, an insecticide currently contaminating the James River Estuary, as the tracer for our study because it primarily associates with organic matter in sediments, does not readily degrade or volatilize in sterile systems and is found associated almost entirely with sediments in the field [9–16].

MATERIALS AND METHODS

Experimental Methods

Continuous-flow experimental systems (Fig. 1) were constructed as previously described by O'Neill et al. [16]. They consisted of four 3-liter reaction kettles (Pyrex Glass Co., Corning, NY), 25 cm deep and 13 cm in diameter, each containing a sediment bed (8 cm deep) covered with 1,500 ml of seawater. Sediment was collected from Pensacola Bay (Pensacola, FL) with an Eckman dredge. The sediment slurry was sieved through a 2-mm Nitex (Tetko, Elmsford, NY) screen and equal volumes of the slurry were added to each vessel. Special care was taken to ensure that each system received the same volume and particle-size distribution of sediment. We added formaldehyde (5%, v/v) to sterilize the systems. No viable cells (as measured by standard plate counts) were detected shortly after the addition of the formaldehyde. Sediment in the vessels was allowed to settle for 7 d prior to the addition of Kepone. A control system contained only water (no sediment).

A glass rod (0.5 cm × 8.0 cm long, with the last 1.0 cm bent at a 120° angle) attached to the shaft of a constant revolution (300 rpm) electric motor

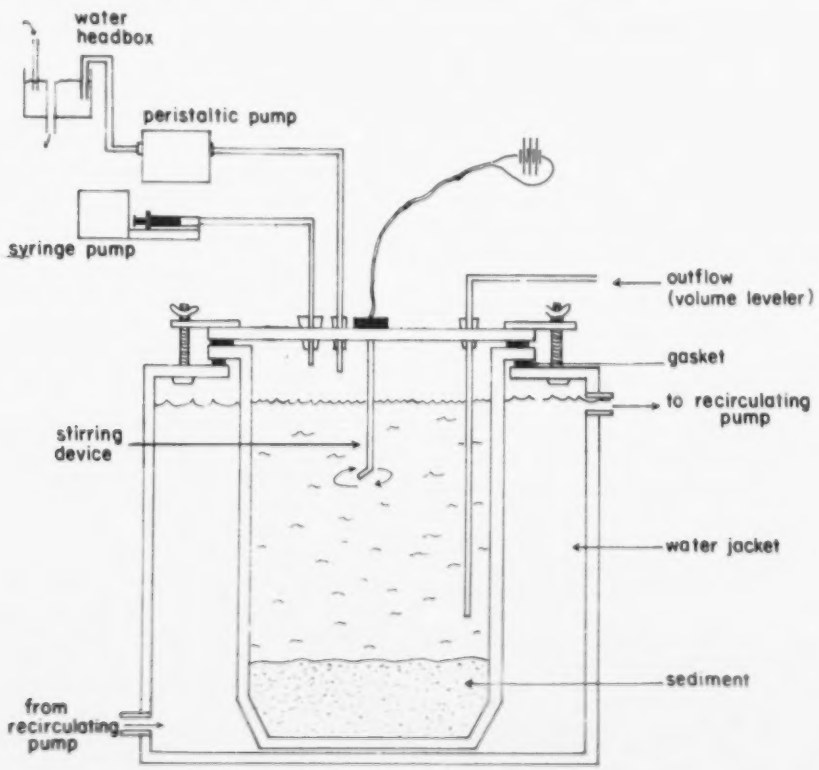

Fig. 1. Sediment-water system.

(Hurst, Princeton, IN) continuously mixed the water column without visibly disturbing the sediment-water interface. The water level in each vessel was maintained by a siphon, and a circulating bath (Neslab Instrument Co., Portsmouth, NH) kept the vessels at a constant temperature of 20°C.

Seawater (20 to 25‰), prefiltered through coarse sand and 20-μm filter cartridges (Brunswick, Timonium, MD), was continuously pumped into each vessel. A peristaltic pump (Harvard Apparatus Co., Millis, MA) delivered the seawater through silicone tubing (wrapped with aluminum foil) at 40 ml/h, producing a retention time of 37.5 h.

[U-^{14}C]Kepone (decachloro-octahydro-1,3,4-metheno-2H-cyclobuta[cd]-pentalen-2-one, 24.8 mCi/mM; Pathfinder Laboratories, St. Louis, MO), was introduced with a syringe pump (Harvard Apparatus Co., Millis, MA) into the vessels through Teflon tubing at a rate of 0.10 ml/h. Continuous input of Kepone was necessary to obtain significant concentrations of the chemical with depth in the sediment. Formaldehyde was added weekly to each vessel. Temperature, pH and salinity were recorded daily.

Kepone concentration in the water overlying the sediment was determined from changes in total radioactivity. Three-milliliter samples from the water column were placed in PCS scintillation cocktail (Amersham Corp., Arlington Heights, IL) and the radioactivity was measured with a scintillation counter (Beckman LS8100; Beckman Instruments, Fullerton, CA). Counts were corrected for background and quenching. Because Kepone does not degrade, distribution of total radioactivity could be used as a direct measure of Kepone distribution. The volume and radioactivity of effluents from the vessels were measured daily.

The sediment was fractionated and analyzed [16] to determine the distribution of Kepone in sediment after 100, 300, 600 and 1,200 h. The thickness of each of the top two layers was less than 1.0 cm, while the bottom four layers ranged in thickness from 1.0 to 3.0 cm. The volume of interstitial water associated with the sediment was measured and the radioactivity in a 3-ml sample was determined. This radioactivity represented the dissolved Kepone concentration in the interstitial water. The sediment was dried to a constant weight at 105°C. Triplicate subsamples (0.5 g) of the dried sediment were analyzed for radioactivity by combustion in a sample oxidizer (Packard B306; Downers Grove, IL). This radioactivity represented sorbed Kepone concentrations.

Moisture content was calculated from differences in the wet and dry weights of each sediment layer [17]. This volume was added to the interstitial water volume for calculations of the total water volume of each layer. The concentration of chemical in the sediment water was insignificant and was not added to the concentration on the sediment (Table 1). Porosity was calculated from the ratio of total water volume to the dimensional volume of the layer. Organic matter content (mg/g) of each sediment layer was determined by the weight lost on combustion (550°C for 30 min) [17]. The concentration of sand (mg/g of sediment) was determined for each sediment layer [17].

On completion of the experiment, vessels, effluent containers and glass tubing were rinsed with acetone. The acetone was then analyzed for radioactivity.

The sorption rate and equilibrium partition coefficient for Kepone were determined in 2-liter flasks containing 500 ml of filtered (3-μm cellulose acetate filter; Nuclepore, Pleasanton, CA) seawater and 250 mg (dry weight) of sediment. Radiolabeled Kepone in acetone was added to an empty flask to give a final concentration of 200 ppb. The acetone was evaporated under a stream of nitrogen and the appropriate amount of filtered seawater was added to the flask. The solution was stirred with a magnetic stirrer until a constant concentration of Kepone was obtained. This solution (200 ppb) was added to each test flask along with a sediment slurry (500 mg/L final concentration). Formaldehyde (2%, v/v) was added and the suspensions were continuously mixed on a shaker table at 125 rpm.

The sorption rate of Kepone to the sediment was measured from the decrease in concentration

Table 1. Budget of total radioactivity (Kepone distribution as percentage of total radioactivity)

Source of radioactivity	Duration of test (h)			
	100	300	600	1,200
Water column	28.7	9.5	5.4	6.8
Sediment	19.4	14.4	11.8	9.4
Interstitial water	0.1	0.2	0.2	0.1
Effluent	48.1	67.1	68.9	78.3
Rinses	1.5	3.5	2.5	2.0
Samples[a]	0.3	0.5	0.3	0.3
Total	98.1	95.2	89.1	96.9

[a]Total of daily samples.

of radioactivity in the water (after removal of sediment by centrifugation, 10 min at 800 *g*). The equilibrium partition coefficient (micrograms sorbed chemical per kilogram organic matter divided by the micrograms dissolved chemical per liter water) was calculated after the concentration of radioactivity in the water became relatively constant. Sorbed Kepone in the sediment was extracted with acetonitrile and the radioactivity of the extract was determined. Budgets of radioactivity averaged 98%.

The radiochemical purity of Kepone was determined to be 85% by high-pressure liquid chromatography (Waters Co., Milford, MA). Kepone was separated on an 8C-18, 10-μm Radial PAK A column with an acetonitrile:phosphate buffer (0.01 M KH_2PO_4, pH 1.95) mobile phase (50:50, v/v) and resolved at a flow rate of 3 ml/min. Kepone was detected by UV absorbance at 254 nm.

Theory

The concentration of chemical in the water column and sediment of the laboratory system is given by a mass balance for each of the segments into which the system is divided (Fig. 2).

Mass balance equations were written for dissolved and adsorbed chemical. The equations were simplified by assuming that the adsorption/desorption reaction was in local equilibrium. This assumption is valid if the adsorption reaction is rapid relative to all other processes. The equations are expressed in terms of the total concentration of chemical:

$$c_t = \Phi c + p \qquad (1)$$

where c_t is the total concentration of chemical (μg/L of segment volume), Φ is the porosity, c is the concentration of dissolved chemical (μg/L of

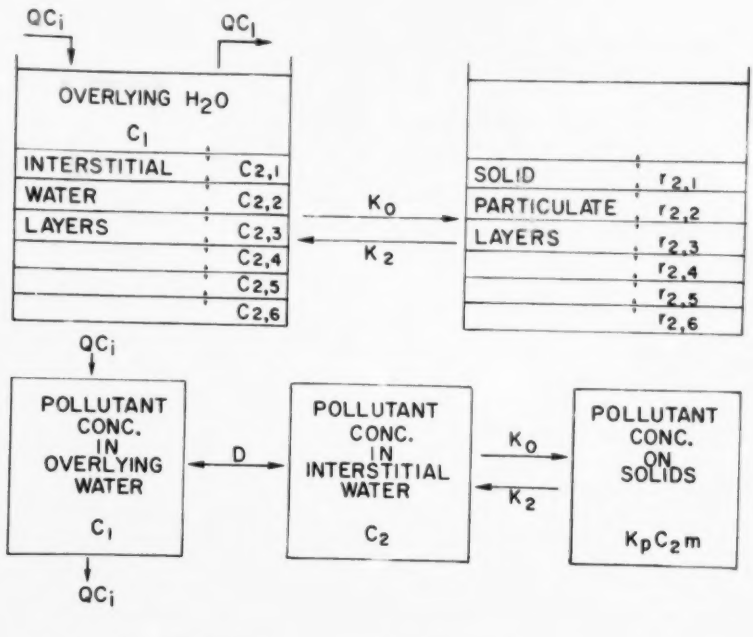

Fig. 2. Diagram of model structure.

interstitial water) and p is the concentration of sorbed chemical (μg/L of segment volume). If several solids types are considered, then

$$c_t = \Phi c + \sum_{i=1}^{n} p_i \tag{2}$$

The concentration of sorbed chemical is determined from the concentration of the solids by

$$p = rm \tag{3}$$

where r is the mass of chemical sorbed per mass of solids (μg/g) and m is the concentration of solids (g/L of total volume).

Equation 2 may therefore be written as

$$c_t = \Phi c + \sum_{i=1}^{n} r_i m_i \tag{4}$$

If adsorption equilibrium is assumed, the relationship between the dissolved chemical concentration and the mass concentration of adsorbed chemical r is specified by the sorption isotherm. For most chemicals, the isotherm is linear at a constant solids concentration and is expressed in terms of a partition coefficient, k_p:

$$r = k_p c \tag{5}$$

The partition coefficient is defined as the weight of chemical sorbed per weight of solids divided by the mass of chemical in solution per volume of solution at equilibrium. The partition coefficient can also be defined in terms of organic carbon content rather than solids. Then the units of r and m would be grams of organic matter per liter of segment volume and micrograms per gram organic matter, respectively. Combining Equations 4 and 5, the total sorbed concentration may be written as

$$c_t = c[\Phi + \Sigma k_{p_i} m_i] \tag{6}$$

The fraction of the total concentration of the chemical that is dissolved, f_d, may be written as

$$f_d = \frac{c}{c_t} = \frac{1}{\Phi + \Sigma k_{p_i} m_i} \tag{7}$$

Similarly, the fraction of total concentration of chemical adsorbed to a particular solids type j, f_{p_j}, is given as

$$f_{p_j} = \frac{p_j}{c_t} = \frac{k_{p_j} m_j}{\Phi + \Sigma k_{p_i} m_i} \tag{8}$$

It is evident from Equations 7 and 8 that the distribution of the dissolved and sorbed components may be determined directly from the distribution of the total concentration of the chemicals and the concentration of solids (organic matter).

The mass balance equation describing total chemical concentration in the water column in our test system is

$$V_1 \frac{dc_1}{dt} = Qc_i - Qc_1 + E_{1,2}(f_{d_2} c_{t_2} - f_{d_1} c_{t_1}) - R_1 \tag{9}$$

where the subscripts 1 and 2 designate the water column and the top sediment layer, respectively; V_1 is the water volume (L); Q is the flow rate (L/h); c_i is the inflow toxicant concentration; $E_{1,2}$ is the exchange coefficient (L/h) between the water column and the interstitial water of the top sediment layer; and R represents the kinetic terms for the applicable individual fate processes. The exchange coefficient is the product of the diffusion coefficient and the sediment surface area divided by the length between the centroids of the water column and top sediment layer:

$$E_{1,2} = \frac{DA}{L_{1,2}} \tag{10}$$

where D is the diffusion coefficient (cm^2/s), A is the sediment surface area (cm^2) and $L_{1,2}$ is distance between the centroids of segments 1 and 2 (cm). The equation for each sediment layer has the form

$$V_n \frac{dc_{t_n}}{dt} = E_{n-1,n}(f_{d_{n-1}} c_{t_{n-1}} - f_{d_n} c_{t_n}) - E_{n,n+1}(f_{d_n} c_{t_n} - f_{d_{n+1}} c_{t_{n+1}}) - R_n \tag{11}$$

In our study with Kepone, the reaction term R is zero because losses from hydrolysis, biodegradation, volatilization, photolysis or other fate processes are negligible.

RESULTS

The sorption rate of Kepone to sediment in the flask studies was rapid, reaching 75% of the equilibrium concentration within 10 min. The equilib-

rium partition coefficient, k_p, was determined to be 8,200 μg/kg (μg/L)$^{-1}$.

When Kepone was continuously introduced into a vessel without sediment, the Kepone concentration in the water showed a rapid increase over the first 100 h and reached the concentration in the inflow water after 250 h (Fig. 3). When Kepone was continuously introduced into systems containing water overlying an undisturbed sediment bed, the Kepone concentration in the water columns increased rapidly during the initial 100 h of the experiment and less dramatically during the next 150 h (Fig. 4). Ultimately, the measured Kepone concentration reached 87% of the inflow water concentration of 16.5 ppb. The presence of sediment, therefore, was largely responsible for the delay in reaching steady-state values. Observed fluctuations in the Kepone concentrations measured in the water columns appeared to be related to inconsistencies in the input of Kepone.

The first sediment layer (thickness approximately 0.3 to 0.6 cm) contained most of the sorbed Kepone; the second sediment layer (thickness approximately 0.3 to 0.9 cm) contained considerably less (Fig. 5). Kepone concentrations in the deeper layers were negligible. Most of the Kepone was recovered in either the sediment, the overlying water or the effluent (Table 1).

The model was initially applied to the system without sediment. The model accurately calculated the observed changes in dissolved Kepone concentration (Fig. 3). The system hydraulics were also described adequately, confirming that no unconsidered sinks, such as volatilization, degradation or wall adsorption, significantly affected Kepone distribution.

The model then was used to quantitate the rate of transport of Kepone from the water column to the sediment. Using the partition coefficient determined in the flask study and the measured porosity and organic matter of the sediment (Table 2), the concentrations of Kepone in the water column and sediment were calculated for two transport scenarios: (a) molecular diffusion between water column and sediment and within sediment, and (b) turbulent diffusion between water column and sediment, decreasing to molecular diffusion with depth in the sediment.

The molecular diffusion coefficient, 3.55×10^{-6} cm^2/s, was calculated from an empirical relationship between molecular weight and diffusivity:

$$D = 22M^{-2/3} \times 10^{-5}$$

where D is diffusion in water and M is molecular weight. This value was close to the diffusion coefficient of 3.87×10^{-6} cm^2/s calculated by the method of Hayduk and Laudie [18]. Diffusion into and within the sediment bed (bulk sediment diffusion) is less than diffusion in free solution. The difference is due to the distance a chemical must travel around a sediment particle (tortuosity) and the number of particles the chemical encoun-

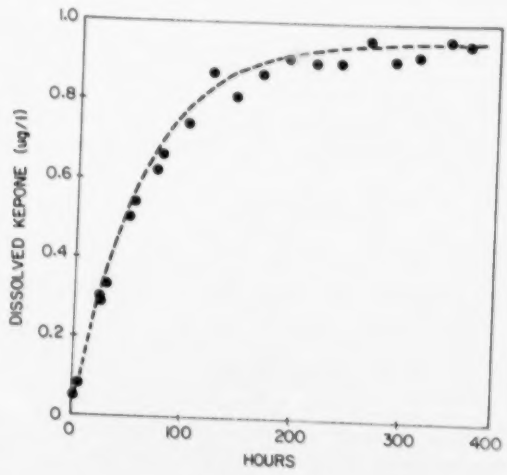

Fig. 3. Observed Kepone concentrations in water system (inflow concentration 0.96 μg/L) without sediment (•), and the model calculation (---).

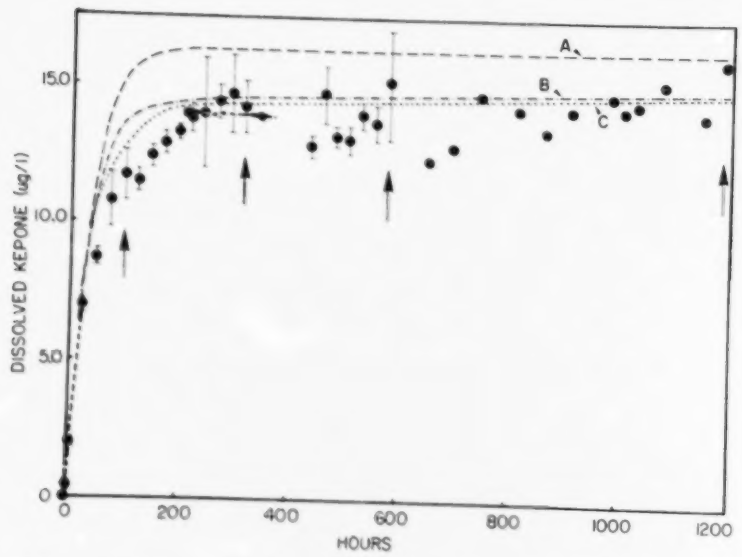

Fig. 4. Observed Kepone concentrations (•) in water column (inflow cncentration 16.5 μg/L) of four systems containing sediment. Arrows indicate end of measurement for a system. The model calculations were obtained with different diffusion coefficients: (A) bulk diffusion (taken from the literature, 2.6×10^{-6} cm^2/s); (B) turbulent diffusion (7.0×10^{-5} cm^2/s, water column into first sediment layer; 5.0×10^{-6} cm^2/s, first sediment layer into second layer); (C) turbulent diffusion decreased over time (see Fig. 7).

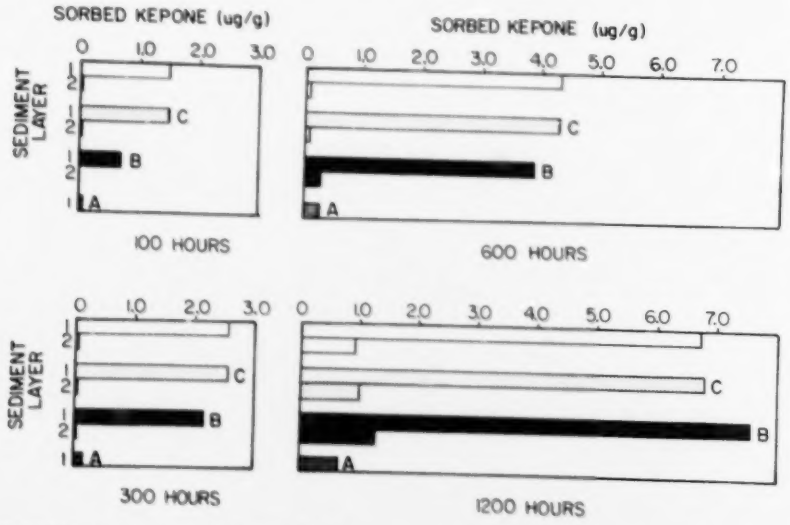

Fig. 5. Observed Kepone concentration (open bar) in upper two sediment layers and model calculations with bulk sediment diffusion coefficient (A), turbulent diffusion coefficient (B) and decreasing turbulent diffusion coefficient over time (C). See Figure 4 for values.

Table 2. Organic matter and porosity values for each sediment-water system

Sediment layer	Duration of test (h)			
	100	300	600	1,200
Organic matter (mg/g)				
1	148	131	160	144
2	147	129	156	115
3	134	123	155	120
4	129	95	134	113
5	121		148	123
6	108		120	108
Porosity				
1	0.883	0.887	0.906	0.860
2	0.857	0.848	0.889	0.834
3	0.833	0.818	0.873	0.782
4	0.820	0.738	0.863	0.780
5	0.811		0.861	0.766
6	0.745		0.827	0.748

ters (porosity). The effect of tortuosity on diffusion can be expressed as

$$D_s = D_o/\theta^2$$

where D_s is the bulk sediment diffusion, D_o is the free solution diffusion coefficient and θ is the geometric tortuosity [19]. The term θ^2 can be related to sediment porosity (Φ) and the formation resistivity factor (F) [20] by

$$\theta^2 = \Phi F$$

In cases in which F cannot be measured, an empirical relationship to porosity can be used [21]:

$$F = \frac{1}{\Phi^m}$$

where the exponent m is equal to 3 for porosities of approximately 0.7 or greater and is equal to 2 for porosities of approximately 0.7 or less [22]. Based on these relationships and an average porosity value of 0.870 (typical of our sediment), the bulk sediment diffusion rate was calculated to be 2.6×10^{-6} cm^2/s.

Molecular diffusion provided insufficient transport between the water column and the sediment bed and between the top two sediment segments. Computed concentrations (chi-square analysis at the 95% confidence level) were higher than observed in the water column (Fig. 4, curve A) and lower than observed in the bed (see A, Figs. 5 and 6). An improved fit to the observed data was obtained with a diffusion coefficient between the water column and bed of approximately 30 times molecular diffusion (7.0×10^{-4} cm^2/s) and between the top two sediment layers of approximately 5 times molecular diffusion (5.0×10^{-6} cm^2/s) (see B, Figs. 4, 5 and 6). If the diffusion rate between the water column and the sediment is decreased over time, computed concentrations fit the data better than is possible with a temporally constant value (see C, Figs. 4, 5 and 6).

To check whether differences between observed and computed values could have been the result of

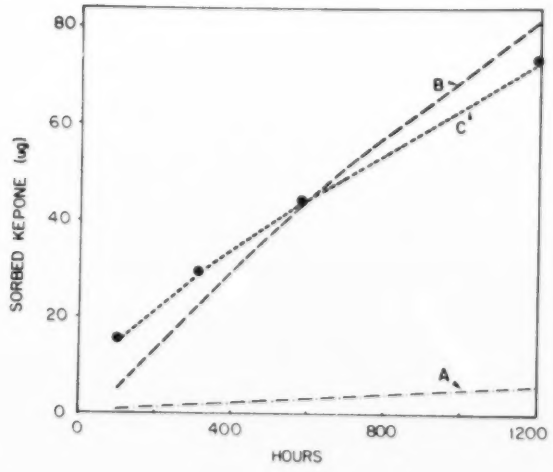

Fig. 6. Total sorbed Kepone observed in the sediment (●) and model calculations with bulk sediment diffusion coefficient (A), turbulent diffusion coefficient (B) and decreasing turbulent diffusion coefficient over time (C). See Figure 4 for values.

a poor estimate of k_p, the value of k_p was varied and the calculated concentrations were evaluated.

DISCUSSION

Kepone accumulated in the top-most layer of an undisturbed sediment bed. Partitioning was high enough to prevent significant penetration of the chemical into the sediment. Although this effect of partitioning on the distribution of a hydrophobic chemical in sediment is expected, the effect has rarely been demonstrated in laboratory experiments or in estuarine sediments taken from the field. Kepone concentrations measured in sediment cores taken from the James River were shown by Huggett et al. [9] to extend below a 60-cm depth. Based on our results and model simulations of the James River, Kepone would never reach these depths by diffusion and partitioning alone. Other factors such as sedimentation, sediment mixing, resuspension and/or dilution with uncontaminated sediments would account for this penetration into the sediment bed. Connolly [10] showed, in a laboratory system designed to systematically resuspend sediments from a sediment bed, that Kepone distribution in a sediment bed can be changed depending on the extent of sediment resuspension.

Huggett et al. [9] also observed, at several sites, significantly higher concentrations of Kepone among upper sediment layers in samples from depths of 10 to 20 cm. Such "banding" could result from initial accumulation of Kepone at the sediment surface, as observed in our experiments, followed by deposition of new sediment that buries the Kepone-contaminated sediment. Soil leaching studies have shown that hydrophobic pesticides accumulate in the top layer of soil columns and are essentially immobilized. Felsot et al. [22], for example, in studies of the vertical disribution of terbufos, a hydrophobic organophosphate insecticide, in soil columns, showed that more than 90% of the terbufos was recovered in the top 6.0 cm of soil despite extensive leaching by rainwater.

Our attempts at computing the observed movement and distribution of Kepone in a static sediment bed revealed that we lacked adequate information on diffusion coefficients for Kepone movement in sediments. The use of a calculated molecular diffusion coefficient taken from the literature resulted in calculated concentrations that greatly underestimated concentrations of Kepone observed in the sediments. Increasing diffusion rates in the model gave a more accurate simulation of the experimental results. High rates of diffusion from the water column into the interstitial water of the top sediment layer are reasonable because of turbulence created from mixing in the water column.

In our systems, the water column was stirred as fast as possible without visibly resuspending sediment. The resulting turbulence apparently increased mixing of the pore water [21,23] and enhanced the diffusion of Kepone. This is the same type of mixing (but not the same magnitude) that occurs in sediments in estuaries and salt marshes as a result of current, tidal, wave and wind actions [20] and bioturbation [16,21,24]. Because little modeling of these mixing processes in shallow water systems (both laboratory and field) has been done, most investigators treat the processes stochastically in terms of an increased "diffusion" rate rather than an increase in an advective flow [20,22,24]. Thus diffusion coefficients encompass both biological-hydrodynamic mixing and molecular diffusion.

A specific example of this approach was reported by Hesslein [23]. To model mathematically the observed concentrations of tritium in the top 10 cm of lake sediments during autumn turnover, he arbitrarily increased the bulk sediment diffusion coefficient of approximately 2.5-fold on the assumption that an increase in mixing of the interstitial water had occurred, possibly due to a convective turnover of pore water. We have used the same logic in modeling our data. The water turbulence in our laboratory systems necessitated an increase in the bulk sediment diffusion coefficient of approximately 30-fold.

A larger bulk sediment diffusion coefficient again was required in predicting the observed movement of Kepone from the first sediment layer to the second layer, probably because of pore-water mixing. Increased depth in the sediment would reduce the effects of turbulence in the water column, thus, explaining why only a five fold increase in the bulk diffusion coefficient was necessary.

Pore-water mixing should continue to decrease with depth in the sediment. However, because Kepone did not move into these lower layers, estimations of diffusion rates with the model were not possible. At the depth in the sediment bed at which pore-water mixing is negligible, porosity and tortuosity would become major factors controlling diffusion. Diffusion coefficients similar to our calculated bulk sediment diffusion coefficient should

then adequately predict the distribution of a chemical at these lower depths.

It is possible that the surface of the sediment bed sorbed significant quantities of Kepone independently of diffusion processes. Sorption of Kepone below the sediment surface presumably would be diffusion dependent. The surface microlayer would continue to come to equilibrium with any increases in concentration of Kepone in the water column until all of the sorptive sites were effectively saturated. At saturation, Kepone removal from the water column would depend on sorptive sites below the microlayer and the diffusion rate to those sites. The microlayer adsorption would, therefore, be time dependent and would effectively place more Kepone in the sediment than expected, particularly upon first exposure. The use of a diffusion coefficient that decreased over time in the model accounted for possible microlayer effects. We estimate that effective saturation of the microlayer in our test system occurred at around 600 h. Diffusion of Kepone across the sediment-water interface, excluding the microlayer effect, was, therefore, approximately 6 to 7 $\times 10^{-5}$ cm^2/s at all times (Figs. 6 and 7).

Our test systems proved adequate for assessing the movement of Kepone, a hydrophobic chemical, across a sediment-water interface and for assessing the distribution of Kepone in the underlying bed. Application of a mathematical model to the observed data indicated that the equilibrium partition coefficient derived from batch experiments was of the correct magnitude. Our results further suggest that molecular diffusivities of organic compounds in water are inappropriate for describing movement in a system containing a static sediment bed.

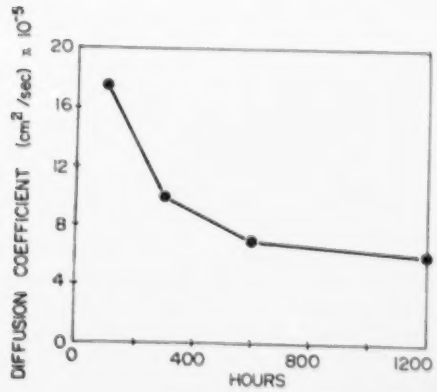

Fig. 7. Model calculation of turbulent diffusion coefficients over time for Kepone movement from the water to the top sediment layer.

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